

Hyperfine structure splitting of the ground states in the $pd\mu$, $pt\mu$ and $dt\mu$ ions

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Abstract

The hyperfine structure splittings of the ground states of the $pd\mu$, $pt\mu$ and $dt\mu$ ions are determined with the use of highly accurate expectation values of the interparticle delta-functions obtained in recent computations. The corresponding hyperfine structure splittings, e.g., $\Delta_{12} = 1.3400149 \cdot 10^7$ MHz and $\Delta_{23} = 3.3518984 \cdot 10^7$ MHz for the $pt\mu$ ion, can directly be measured in modern experiments.

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In this study we analyze the hyperfine structure and determine the hyperfine structure splitting of the bound $S(L = 0)$ -states in the non-symmetric muonic molecular ions $pd\mu$, $pt\mu$ and $dt\mu$. As is well known there are four bound $S(L = 0)$ -states in these three ions: three ground $S(L = 0)$ -states (one in each of these ions) and one excited $S(L = 0)$ -state in the heavy $dt\mu$ ion. In this study we want to investigate the hyperfine structure and determine the hyperfine structure splittings for each of these bound states by using highly accurate expectation values of the delta-functions obtained in recent highly accurate numerical computations.

The general formula for the hyperfine structure splitting $(\Delta H)_{h.s.}$ (or hyperfine splitting, for short) for an arbitrary three-body system is written as the sum of the three following terms. Each of these terms is proportional to the product of the factor $\frac{2\pi}{3}\alpha^2$ and expectation value of the corresponding (interparticle) delta-funtion. The third (additional) factor contains the corresponding g -factors (or hyromagnetic ratios) and scalar product of the two spin vectors. For instance, for the $pd\mu$ ion this formula takes the form (in atomic units) (see, e.g., [1], [2])

$$(\Delta H)_{h.s.} = \frac{2\pi}{3}\alpha^2 \frac{g_p g_d}{m_p^2} \langle \delta(\mathbf{r}_{pd}) \rangle (\mathbf{s}_p \cdot \mathbf{s}_d) + \frac{2\pi}{3}\alpha^2 \frac{g_p g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{p\mu}) \rangle (\mathbf{s}_p \cdot \mathbf{s}_\mu) + \frac{2\pi}{3}\alpha^2 \frac{g_d g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{d\mu}) \rangle (\mathbf{s}_d \cdot \mathbf{s}_\mu) \quad (1)$$

where $\alpha = \frac{e^2}{\hbar c}$ is the fine structure constant, m_μ and m_p are the muon and proton masses, respectively. The factors g_μ , g_p and g_d are the corresponding g -factors. The expression for $(\Delta H)_{h.s.}$ is, in fact, an operator in the total spin space which has the dimension $(2s_p + 1)(2s_d + 1)(2s_\mu + 1) = 12$. In our calculations we have used the following numerical values for the constants and factors in Eq.(1): $\alpha = 7.297352586 \cdot 10^{-3}$, $m_p = 1836.152701m_e$, $m_\mu = 206.768262m_e$ and $g_\mu = -2.0023218396$. The g -factors for the proton and deuteron are deteremined from the formulas: $g_p = \frac{\mathcal{M}_d}{I_p}$ and $g_d = \frac{\mathcal{M}_d}{I_d}$, where $\mathcal{M}_p = 2.792847386$ and $\mathcal{M}_d = 0.857438230$ are the magnetic moments (in nuclear magnetons) of the proton and deuteron, respectively. The spin of the proton and deuteron is designated in Eq.(1) as $I_p = \frac{1}{2}$ and $I_d = 1$.

The analogous formula for the hyperfine structure splitting in the $pt\mu$ ion takes the form

$$(\Delta H)_{h.s.} = \frac{2\pi}{3}\alpha^2 \frac{g_p g_t}{m_p^2} \langle \delta(\mathbf{r}_{pt}) \rangle (\mathbf{s}_p \cdot \mathbf{s}_t) + \frac{2\pi}{3}\alpha^2 \frac{g_p g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{p\mu}) \rangle (\mathbf{s}_p \cdot \mathbf{s}_\mu)$$

$$+ \frac{2\pi}{3} \alpha^2 \frac{g_t g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{t\mu}) \rangle (\mathbf{s}_t \cdot \mathbf{s}_\mu) \quad (2)$$

where $g_t = \frac{\mathcal{M}_t}{I_t}$, where $\mathcal{M}_t = 2.9789624775$ is the magnetic moment of the triton expressed in the nuclear magnetons and $I_t = \frac{1}{2}$ is the spin of the triton (or tritium nucleus). The formula for the hyperfine structure splitting in the $dt\mu$ ion is

$$\begin{aligned} (\Delta H)_{h.s.} = & \frac{2\pi}{3} \alpha^2 \frac{g_d g_t}{m_p^2} \langle \delta(\mathbf{r}_{dt}) \rangle (\mathbf{s}_d \cdot \mathbf{s}_t) + \frac{2\pi}{3} \alpha^2 \frac{g_d g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{d\mu}) \rangle (\mathbf{s}_d \cdot \mathbf{s}_\mu) \\ & + \frac{2\pi}{3} \alpha^2 \frac{g_t g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{t\mu}) \rangle (\mathbf{s}_t \cdot \mathbf{s}_\mu) \end{aligned} \quad (3)$$

where all values are defined above. The same formula can be applied to determine the hyperfine structure splittings in the excited $S(L = 0)$ -state of the $dt\mu$ ion. The only difference in the hyperfine structure splittings determined for the ground and excited states of the $dt\mu$ ion can be related with the expectation values of interparticle delta-functions.

In our computations of the muonic molecular ions performed recently [3] we have determined the expectation values of all delta-functions which are needed in Eqs.(1) - (3). The corresponding expectation values are shown in Table I. These values have been determined in muon atomic units where $m_\mu = 1, \hbar = 1, e = 1$. They must be re-calculated to the regular atomic units ($m_e = 1, \hbar = 1, e = 1$) which are used in the formulas, Eqs.(1) - (3), to determine the hyperfine structure splittings. In these calculations we have used the trial wave functions with $N = 3300, 3500, 3700$ and 3840 exponential basis functions (for more details, see [3]). The expectation values of all interparticle delta-functions computed for the ground $S(L = 0)$ -state of the $pd\mu$ ion are shown in Table I. The overall convergence rates of the delta-functions computed for each bound state in the $pt\mu$ and $dt\mu$ ions are very similar to the results shown in Table I.

These expectation values of the $\delta(\mathbf{r}_{ij})$ -functions were used in the formulas Eqs.(1) - (3) to determine the hyperfine structure splittings of the bound $S(L = 0)$ -states of the $pd\mu, pt\mu$ and $dt\mu$ ions. Numerical values of the corresponding hyperfine structure splittings can be found in Tables II and III. Note that these values are usually given in MHz , while the values of $(\Delta H)_{h.s.}$ which follow from Eqs.(1) - (3) are expressed in atomic units. To re-calculate them from atomic units to MHz the conversion factor $6.57968392061 \cdot 10^9 \text{ MHz}/a.u.$ was used [4].

In general, the $pd\mu$ and $dt\mu$ ions have similar hyperfine structure. In particular, in each of these ions one finds twelve spin states which are separated in the four following groups:

(1) the group with $J = 2$ (five states), (2) the group with $J = 1$ (three states), (3) the group of one state with $J = 0$ (one state) and (4) the group with $J = 1$ (three states). Here and everywhere below the notation J stands for the total spin (or total momentum, for the $S(L = 0)$ -states) of the three-body ion. The states with $J = 2$ have the maximal energy, while the energy of the states from the fourth group is minimal. The corresponding splittings Δ_{12}, Δ_{23} and Δ_{34} can be found in Table II for each bound state in the $pd\mu$ and $dt\mu$ ions.

The hyperfine structure of the ground state in the $pt\mu$ ion is completely different (see Table III) from the hyperfine structures of the $pd\mu$ and $dt\mu$ ions discussed above. It follows from the fact that the spin of the triton equals $\frac{1}{2}$, while the spin of the deuteron (or deuterium nucleus) equals 1. In the case of the ground state in the $pt\mu$ ion one finds only eight spin states which are separated into three different groups: (1) the group of four states with $J = \frac{3}{2}$, (2) the group of two states with $J = \frac{1}{2}$ and (3) the group of two states with $J = \frac{1}{2}$. The group (1) has the maximal energy, while the energy of the states from the third group is minimal. The corresponding values of the hyperfine structure splittings in the ground state of the $pt\mu$ ion are $\Delta_{12} = 1.3400149 \cdot 10^7 \text{ MHz}$ and $\Delta_{23} = 3.3518984 \cdot 10^7 \text{ MHz}$.

Thus, we have determined the hyperfine structure splitting in the bound $S(L = 0)$ -states of the $pd\mu, pt\mu$ and $dt\mu$ ions. The hyperfine structure splitting of the first excited $S(L = 0)$ -state in the $dt\mu$ ion is considered too. This excited state is traditionally designated by an additional asterisk, i.e. $(dt\mu)^*$. In our calculations we used the highly accurate expectation values of all interparticle delta-functions obtained in recent computations [3]. In general, it is very interesting to compare the numerical values of the hyperfine structure splittings Δ_{12}, Δ_{23} and Δ_{34} determined for the different muonic ions (see Table II).

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TABLE I: The convergence of the $\langle\delta_{32}\rangle$, $\langle\delta_{31}\rangle$ and $\langle\delta_{21}\rangle$ expectation values for the ground (bound) $S(L=0)$ -state of the $pd\mu$ molecular ion (in muon-atomic units).

N	$\langle\delta_{32}\rangle$	$\langle\delta_{31}\rangle$	$\langle\delta_{21}\rangle$
3300	$1.73456203087\cdot 10^{-1}$	$1.17709732798\cdot 10^{-1}$	$1.46169407\cdot 10^{-5}$
3500	$1.73456202965\cdot 10^{-1}$	$1.17709733128\cdot 10^{-1}$	$1.46169370\cdot 10^{-5}$
3700	$1.73456202754\cdot 10^{-1}$	$1.17709733014\cdot 10^{-1}$	$1.46169377\cdot 10^{-5}$
3840	$1.73456202768\cdot 10^{-1}$	$1.17709733160\cdot 10^{-1}$	$1.46169383\cdot 10^{-5}$

TABLE II: The levels of hyperfine structure ϵ and hyperfine structure splittings Δ in the bound $S(L=0)$ -states of the $pd\mu$ and $dt\mu$ ions (in MHz).

$\epsilon_{J=2}(pd\mu)$	$1.2519350851\cdot 10^7$	—	—
$\epsilon_{J=1}(pd\mu)$	$9.3058194294\cdot 10^6$	$\Delta(J=2 \rightarrow J=1)$	$3.2135314217\cdot 10^6$
$\epsilon_{J=0}(pd\mu)$	$-2.1222395094\cdot 10^7$	$\Delta(J=1 \rightarrow J=0)$	$3.0528214524\cdot 10^7$
$\epsilon_{J=1}(pd\mu)$	$-2.3097272483\cdot 10^7$	$\Delta(J=0 \rightarrow J=1)$	$1.8748773889\cdot 10^6$
$\epsilon_{J=2}(dt\mu)$	$1.8919590437\cdot 10^7$	—	—
$\epsilon_{J=1}(dt\mu)$	$1.5985479092\cdot 10^6$	$\Delta(J=2 \rightarrow J=1)$	$2.9341113453\cdot 10^6$
$\epsilon_{J=0}(dt\mu)$	$-3.4439378258\cdot 10^7$	$\Delta(J=1 \rightarrow J=0)$	$5.0424857350\cdot 10^7$
$\epsilon_{J=1}(dt\mu)$	$-3.6038337067\cdot 10^7$	$\Delta(J=0 \rightarrow J=1)$	$1.5989588085\cdot 10^6$
$\epsilon_{J=2}(dt\mu)^*$	$1.8609555434\cdot 10^7$	—	—
$\epsilon_{J=1}(dt\mu)^*$	$1.6554331952\cdot 10^6$	$\Delta(J=2 \rightarrow J=1)$	$2.0552234821\cdot 10^6$
$\epsilon_{J=0}(dt\mu)^*$	$-3.4859818025\cdot 10^7$	$\Delta(J=1 \rightarrow J=0)$	$5.1414149977\cdot 10^7$
$\epsilon_{J=1}(dt\mu)^*$	$-3.5950318334\cdot 10^7$	$\Delta(J=0 \rightarrow J=1)$	$1.0905003094\cdot 10^6$

TABLE III: The levels of hyperfine structure ϵ and hyperfine structure splittings Δ in the ground $S(L = 0)$ -state of the $pt\mu$ ion (in MHz).

$\epsilon_{J=\frac{3}{2}}(pt\mu)$	$1.5079820356 \cdot 10^7$	—	—
$\epsilon_{J=\frac{1}{2}}(pt\mu)$	$1.6796717260 \cdot 10^6$	$\Delta(J = \frac{3}{2} \rightarrow J = \frac{1}{2})$	$1.3400148630 \cdot 10^7$
$\epsilon_{J=\frac{1}{2}}(pt\mu)$	$-3.1839312439 \cdot 10^7$	$\Delta(J = \frac{1}{2} \rightarrow J = \frac{1}{2})$	$3.3518984165 \cdot 10^7$